Néel order in the two-dimensional $S = \frac{1}{2}$-Heisenberg Model

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The existence of Néel order in the $S = \frac{1}{2}$ Heisenberg model on the square lattice at $T = 0$ is shown using inequalities set up by Kennedy, Lieb and Shastry in combination with high precision Quantum Monte Carlo data.

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The ground state order of quantum spin systems, in particular the issue whether the ground state shows long range magnetic order, has attracted long and continuous interest. For the prototype of spin models, the antiferromagnetic Heisenberg model, the existence of Néel order at low temperatures was proved in the seminal paper of Dyson, Lieb and Simon [1] in 1978 for spin $S \geq 1$ and spatial dimension $d \geq 3$ and also for $S = \frac{1}{2}$ and $d > 3$.

Ten years later Kennedy, Lieb and Shastry [2] showed that also for $S = \frac{1}{2}$ and $d = 3$ Néel order in the ground state exists.

The situation in two dimensions is different and more subtle, since the Mermin-Wagner-Hohenberg theorem forbids Néel order at finite T, leaving open however the possibility of Néel order in the ground state. The existence of Néel order for the two-dimensional model and $S \geq 1$ was shown in [3, 4] and later in [2] by an independent derivation of the relevant inequality at $T = 0$.

However the inequalities sufficient to show Néel order for $S = 1$ in the two-dimensional case are not sufficient to construct an analogous proof for $S = \frac{1}{2}$. Thus the case of $S = \frac{1}{2}$ remains an open problem. Still it is possible to derive inequalities concerning spin-spin correlations at *short* distances [2] which are violated if Néel order is present. That is, with a minimum of numerical information, the question of Néel order in the ground state can be decided.

The issue of this paper is to evaluate the spin-spin correlations of the two-dimensional $S = \frac{1}{2}$ antiferromagnetic Heisenberg model at *short* distances and demonstrate that these results combined with the analytic expressions of [2] show the existence of Néel order in the two-dimensional $S = \frac{1}{2}$ antiferromagnetic Heisenberg model at $T = 0$. Such a study has become possible, due to the developement of high precision Monte-Carlo techniques over the last decade.

In Ref.[2] Kennedy, Lieb and Shastry used data of Gross, Sanchez-Velasco and Siggia [5] for a comparison, however these data clearly deviate from the results presented here. The authors of [5] used a Quantum Monte Carlo method without loop updates and with discrete Trotter time (see below). Their data served only as a crude comparison to extrapolated Lanczos data and data produced by the Neumann-Ulam method, which were the best algorithms to study the properties of the two-dimensional Heisenberg model in 1988. Today modern loop algortihms by far outreach both methods.

As will be shown in the following an accurate evaluation of correlation functions at short distances is possible with modern Quantum Monte Carlo methods, which allow us to compute expectation values at very low temperatures and even though the short distance results have a certain finite size and finite temperature correction, these uncertainties are well controlled and allow to draw definite conclusions.

The approach and intention of this paper is diffrent from a completely numerical evaluation of e.g. the correlation length, which involves a calculation of correlations at *long* distances and an appropriate extrapolation to *infinite* distances, which cannot be used as a proof of long range order in any rigorous sense.

At first sight a "Quantum Monte Carlo algorithm" seems a puzzling concept, since an important step in any Monte-Carlo-method is the evaluation of Boltzmann weights for given energies of the system. For quantum models these energies are hard if not impossible to calculate. A key idea to make Monte Carlo methods applicable to quantum systems is to map the quantum model onto a classical model by introducing an extra dimension, usually referred to as Trotter-time [6].

In the first generation of algorithms this mapping was straightforwardly applied to the quantum Heisenberg model. Though this allowed for a wealth of new studies of the finite temperature properties in one and in particular in two-dimensional systems, these algorithms had two major drawbacks, which became most evident at low temperatures. Firstly the extra Trotter dimension was discretized, introducing the number of time slices as a parameter which had to be eliminated from the final results by an extrapolation. Secondly the update procedure, i.e. the construction of new independent configurations, was done locally. As a consequence one had to move through the lattice site by site several times to obtain a configuration independent of the starting configuration and useful for a new evaluation of an observable.

A first improvement was introduced by the so called loop-algorithms [7], which uses nonlocal updates similar to the Swendsen-Wang algorithm for classical models. A second and important step towards high precision Quantum Monte Carlo techniques were algorithms which work directly in the Euclidian time continuum [8] and require no extrapolation in Trotter time. For the algorithm [9] used for the analysis presented here no approximations enter, and statistical errors are the only source of inaccuracy.

Since this work intends to produce highly accurate

data it seems appropriate to assess the precision of the method by a comparison with exact results. The best candidate for such a comparison are the correlations of one-dimensional systems evaluated by the Bethe-ansatz with almost arbitrary precision up to distance seven [10] and with results for finite chains from Ref.[11]. This is done in the Appendix for chains of 400 sites at T=0.005.

After these introductory remarks we now return to our actual goal, which is the two-dimensional system. Our starting point is a $S=\frac{1}{2}$ Heisenberg model

$$H=\sum_{\substack{<xy>\\ x,y\varepsilon\Lambda}}\vec{S}_x\vec{S}_y \tag{1}$$

with nearest neighbour interaction on a finite square lattice Λ with an even number of sites in every direction and periodic boundary conditions.

The Fourier transform of the spin-spin correlation function at $T=0$ is given by

$$g_q=\langle S_{-q}S_q\rangle=\sum_{x\varepsilon\Lambda}e^{-iqx}\langle S_0^3S_x^3\rangle \tag{2}$$

where

$$S_q=\frac{1}{\sqrt{|\Lambda|}}\sum_{x\varepsilon\Lambda}e^{-iqx}S_x^3. \tag{3}$$

For the corresponding finite temperature expectation value of g_q an upper bound f_q was derived in [1]. The $T=0$ limit of this bound was obtained in Ref.[4] and a direct proof of the bound at $T=0$ was given in [2]. Following the notation and arguments of Kennedy, Lieb and Shastry [2] the inequality for $d=2$ reads

$$g_q\leq f_q \quad \text{for} \quad q\neq Q \tag{4}$$

where $f_q=\sqrt{\frac{e_0E_q}{12E_{q-Q}}}$, $E_q=2-\cos q_1-\cos q_2$, $Q=(\pi,\pi)$ and $-e_0$ is the ground state energy per site of the Heisenberg model Eq.1 on the lattice Λ.

The fundamental idea is, that the existence of Néel order in the limit of infinite system size corresponds to a delta-function in the Fourier transform of the spin-spin correlation g_q at Q. This means, if Eq. 4 is integrated over the whole Brillouin zone one finds in the case of Néel order

$$m^2+\int d^2q\ f_q\geq\int d^2q\ g_q=S(S+1)/3 \tag{5}$$

where m^2 is the coefficient of the delta-function at Q.

If there is no Néel order m^2 is zero. By numerically evaluating the integral over f_q, and by using exact variational upper and lower bounds on the ground state energy $-e_0$ one sees, that the above inequality and its analogon for $d\geq 3$ cannot be fulfilled with $m^2=0$ and $S\geq 1$, which proves Néel order.

Inequalities of type Eq. 5 are not sufficient to prove the existence of a nonzero m^2 for $d=2,3$ and $S=\frac{1}{2}$, but a new relation is obtained by multiplying g_q by $\cos q_i$ and again integrating over the Brillouin zone:

$$\int d^dq\ g_q\ \cos q_i=\langle S_0^zS_{\delta_i}^z\rangle=-e0/3d \tag{6}$$

with i=1,2 for d=2 and i=1,2,3 for d=3 and δ_i the unit vector in i-direction and the value of the ground state energy form Ref.[12] is $e_0=0.669437(5)$.

Carrying out an analogous integral over f_q and using again Eq.4 one finds:

$$\frac{e_0}{3d}\leq-\sqrt{\frac{e_0}{6d}}\int d^dq\sqrt{\frac{E_q}{d^2E_{q-Q}}}\left(\sum_{i=1}^{d}\cos q_i\right)_+ \tag{7}$$

were the f_+ means the positive part of a function, which equals f, when f is positive and is zero otherwise.

Again Eq.7, which is valid if no Néel order exists, was shown to be violated for $d=3$ and $S=\frac{1}{2}$ in Ref.[2] by using bounds on e_0 and thus the existence of Néel order was proved also for $d=3$ and $S=\frac{1}{2}$.

For $S=\frac{1}{2}$ and $d=2$ one cannot construct a contradiction by using only the ground state energy. Here more input from numerical data is needed. This can be incorporated by multiplying g_q by $\cos(mq_i)$ with $m=2,3...$ and again integrating over the whole Brillouin zone:

$$\int d^2q\ g_q\ \cos(mq_i)=\langle S_0^3S_{m\delta_i}^3\rangle \tag{8}$$

with i=1,2.

Next, defining $\bar{g}(n)$ as

$$\bar{g}(n)=\frac{1}{n+1}\sum_{m=0}^{n}(-1)^m\langle S_0^3S_{m\delta_i}^3\rangle \tag{9}$$

and using again inequality 4 one constructs the following relations involving the correlation functions:

$$\begin{aligned}\bar{g}(n)&=\int d^2q\frac{1}{2n+2}\sum_{m=0}^{n}(-1)^m\{\cos(mq_1)+\cos(mq_2)\}\ g_q\\ &\leq\int d^2q\frac{1}{2n+2}\sum_{m=0}^{n}(-1)^m\{\cos(mq_1)+\cos(mq_2)\}_+\ f_q.\end{aligned} \tag{10}$$

Whenever the inequality Eq. 10 is violated for a certain n, a nonzero m^2 multiplying the delta-function at Q is needed and therefore the existence of Néel order is proved.

The $\bar{g}(n)$ as defined in Eq.9 were calculated by the Quantum Monte Carlo method [9]. The results, displayed in table I, show that the $\bar{g}(n)$ calculated by Quantum Monte Carlo cross the bound obtained by integrating over f_q at $n=8$. This is also depicted in Fig. 1. Thus inequality Eq.10 is violated and Néel order must exists in

n	Bound	$T = 0.005$	$T = 0.025$	$T = 0.075$
1	2.297e-01	1.80799e-01 ± 3.63e-06	1.80794e-01	1.80792e-01
2	1.714e-01	1.40308e-01 ± 5.63e-06	1.40302e-01	1.40298e-01
3	1.383e-01	1.17686e-01 ± 6.84e-06	1.17678e-01	1.17670e-01
4	1.166e-01	1.03005e-01 ± 7.67e-06	1.02997e-01	1.02985e-01
5	1.013e-01	9.27815e-02 ± 8.27e-06	9.27743e-02	9.27544e-02
6	8.990e-02	8.52115e-02 ± 8.73e-06	8.52048e-02	8.51770e-02
7	8.107e-02	7.93875e-02 ± 9.10e-06	7.93811e-02	7.93436e-02
8	7.400e-02	7.47551e-02 ± 9.40e-06	7.47496e-02	7.47012e-02
9	6.820e-02	7.09844e-02 ± 9.64e-06	7.09795e-02	7.09191e-02
10	6.334e-02	6.78504e-02 ± 9.85e-06	6.78464e-02	6.77734e-02
11	5.921e-02	6.52055e-02 ± 1.00e-05	6.52021e-02	6.51163e-02
12	5.563e-02	6.29418e-02 ± 1.02e-05	6.29389e-02	6.28404e-02
13	5.252e-02	6.09835e-02 ± 1.03e-05	6.09806e-02	6.08695e-02
14	4.976e-02	5.92718e-02 ± 1.04e-05	5.92692e-02	5.91456e-02
15	4.732e-02	5.77638e-02 ± 1.06e-05	5.77617e-02	5.76255e-02

TABLE I: Bound obtained by integrating numerically over the right hand side of Eq.10 compared with $\bar{g}(n)$ for a 40×40 lattice and different temperatures.

n	Bound	$T = 0.025$	T=0.025 extrapolated
1	2.297e-01	1.80794e-01	1.80791e-01 ± 5.09e-06
2	1.714e-01	1.40302e-01	1.40295e-01 ± 7.87e-06
3	1.383e-01	1.17678e-01	1.17668e-01 ± 9.53e-06
4	1.166e-01	1.02997e-01	1.02983e-01 ± 1.07e-05
5	1.013e-01	9.27743e-02	9.27534e-02 ± 1.15e-05
6	8.990e-02	8.52048e-02	8.51762e-02 ± 1.21e-05
7	8.107e-02	7.93811e-02	7.93428e-02 ± 1.26e-05
8	7.400e-02	7.47496e-02	7.46995e-02 ± 1.30e-05
9	6.820e-02	7.09795e-02	7.09154e-02 ± 1.34e-05
10	6.334e-02	6.78464e-02	6.77663e-02 ± 1.37e-05
11	5.921e-02	6.52021e-02	6.51035e-02 ± 1.39e-05
12	5.563e-02	6.29389e-02	6.28188e-02 ± 1.41e-05
13	5.252e-02	6.09806e-02	6.08346e-02 ± 1.43e-05
14	4.976e-02	5.92692e-02	5.90923e-02 ± 1.45e-05
15	4.732e-02	5.77617e-02	5.75473e-02 ± 1.46e-05

TABLE II: Bound obtained by integrating numerically over the right hand side of Eq.10 compared with $\bar{g}(n)$ extrapolated for N=40,36,32,24 at $T = 0.025$.

the two-dimensional antiferromagnetic Heisenberg model with $S = \frac{1}{2}$ at $T = 0$.

There are three type of corrections to the data of table I, which need to be taken into account, but which, as we shall show in the following, do not change the above conclusion of a crossing of the curves at $n = 8$:

(i) effects of finite temperature,
(ii) effects of the finiteness of the system,
(iii) statistical errors.

In the following we comment on how these corrections modify the data.

(i) The Quantum Monte Carlo data presented are at $T \geq 0.005$. The overall effect of finite temperature is to lower the absolute value of the correlations and therefore also the value of the $\bar{g}(n)$. The effect of finite temperature is to shift the crossing of the bound and $\bar{g}(n)$ to larger n, or eventually to destroy a crossing completely.

The functional dependence of the internal energy $U(T)$, which up to an overall factor $3z$ ($z = 2$ is the coordination number of the two-dimensional square lattice) equals the correlation-function at distance one, has been determined for low T by spin wave theory [13, 14] as

$$U(T) = -e_0 + bT^3. \tag{11}$$

The coefficient is given in [15] as $b = \frac{\zeta(3)}{2e_0\pi} \approx 0.2853626$, so the correction for distance one is $\approx \frac{b}{6}10^{-7}$, which is two orders of magnitude smaller than the statistical error, (see point (iii)).

For distances larger than one, we fitted the data as a function of temperature (taking the exponent of T as fit parameter) for $T = 0.005, 0.025, 0.05, 0.075$ and found the corrections due to finite temperature all of the order of 10^{-5}, which is the order of the statistical error. Therefore we do not give any finite temperature corrections.

(ii) The absolute value of the correlations in the thermodynamic limit are smaller than in systems of finite size. This means that the effect of finite system size is opposite to the effect of temperature. The finite size behaviour of the ground state energy is well studied for the Heisenberg model on the square lattice. Arguments originating from the quantum nonlinear sigma model description [16] of the Heisenberg model to lowest order in system size give

$$-e_0 = -e_0(N) + \frac{c}{N^3}, \quad \text{with} \quad c > 0 \tag{12}$$

where $-e_0(N)$ is the ground state energy of a system of size $N \times N$. Though the corrections are not substantial, they do effect the results, and taking into account, that the finite size errors in contrast to the finite temperature effects, might falsely lead to a crossing, we extrapolated the data for $N = 24...40$ using the functional dependence Eq.12, which we found well satisfied also for larger distances. The results are shown in table II. One sees that the numeric values are changed but the crossing point is still at $n = 8$.

(iii) We compute $\Delta x = \frac{1}{\sqrt{N_{MC}}}\sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ (where the observable x stands for the value of a correlation at a given distance, temperature and system size and N_{MC} is the number of Monte Carlo iterations), which is a reliable estimate for the statistical error of the mean value $\langle x \rangle$, since for the algorithm of Ref.[9] the autocorrelation time is of order one and the Monte Carlo configurations are almost independent. To assess the quality of our error anal-

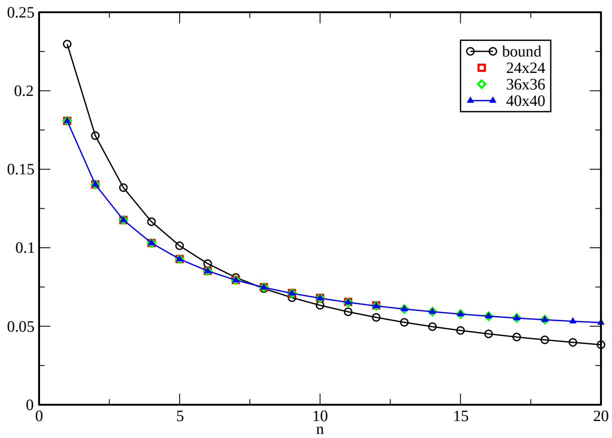

FIG. 1: Bound on $\bar{g}(n)$ obtained from Eq.9 and $\bar{g}(n)$ for 24×24, 36×36 and 40×40 at $T = 0.025$.

Distance	Quantum Monte Carlo	Bethe-Ansatz
0	0.25000000 (0)	
1	-0.14771586 (198)	-0.1477157268
2	0.06067787 (324)	0.0606797699
3	-0.05024194 (282)	-0.0502486272
4	0.03464515 (281)	0.0346527769
5	-0.03088096 (260)	-0.0308903666
6	0.02443619 (255)	0.0244467383
7	-0.02248413 (242)	-0.0224982227
8	0.01895736 (236)	

TABLE III: Correlations for a chain with $N = 400$ sites at T/J=0.005 compared with results from Ref. [10].

ysis we also returned to the case of the one-dimensional antiferromagnetic Heisenberg model (see Appendix) and compared results with independent streams of random numbers.

To calculate an upper limit to the errors of $\bar{g}(n)$, the errors of the correlations where added up (being evaluated with the same configurations, they are not independent).

To conclude, the error analysis shows that the short range correlations entering Eq.9 were determined with sufficiently high accuracy to prove the existence of a crossing of the bound and the Quantum Monte Carlo data for $\bar{g}(n)$ at $n = 8$ and therefore to show the existence of long range order.

Appendix

(1) In this Appendix we list the correlations of a one-dimensional Heisenberg model with periodic boundary conditions and chain length $N = 400$ at T=0.005 compared with results of Ref.[10] for infinite chain length and $T = 0$.

For the internal energy $U(T)$ of the Heisenberg *chain* the temperature dependence for low T is $U(T) = -e_0^1 + aT^2$ with the ground-state energy $e_0^1 = 0.4431471804$ for 400 sites and $e_0^1 = -\frac{1}{4} + \ln 2$ for the infinite size system[17]. and the coefficient $a = \frac{1}{3}$ given in Ref. [18, 19]. This means that the correction for the correlations in tableIII due to finite temperatures are of the order of 10^{-5}.

(2) The exact values of the correlation functions [11, 20] for distance one and two at $T = 0$ for a chain with 400 sites are $\langle S_0^3 S_1^3 \rangle_{400} = -0.147717441765735$ and $\langle S_0^3 S_2^3 \rangle_{400} = 0.0606813790491800$. The above data show that the error analysis concerning statistical errors and finite temperature effects is consistent.

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